

# Non-Hermitian Hamiltonians, Metric, Other Observables and Physical Implications

H.B. Geyer<sup>1,2</sup>, W.D. Heiss<sup>1,2</sup> and F.G. Scholtz<sup>1</sup>

<sup>1</sup>*Institute of Theoretical Physics, University of Stellenbosch,  
7602 Matieland, South Africa*

and

<sup>2</sup>*National Institute for Theoretical Physics (NITheP),  
Stellenbosch Institute for Advanced Study,  
7600 Stellenbosch, South Africa*

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The metric associated with a quasi-Hermitian Hamiltonian and its physical implications are scrutinised. Consequences of the non-uniqueness such as the question of the probability interpretation and the possible and forbidden choices of additional observables are investigated and exemplified by specific illustrative examples. In particular it is argued that the improper identification of observables lies at the origin of the claimed violation of the brachistochrone transition time between orthogonal states. The need for further physical input to remove ambiguities is pointed out.

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## I. INTRODUCTION

Quantum mechanics is formulated within the mathematical framework of a Hilbert space with linear operators acting on the elements of a Hilbert space - the physical state vectors. Traditionally, the linear operators considered are Hermitian operators (in the  $L^2$  or Dirac sense of transposition and complex conjugation), if they describe quantities called (physical) observables<sup>30</sup>. In fact, the mathematical structure of Hermitian operators is well understood in that they guarantee a real spectrum. Of equal importance is the complete and orthogonal eigensystem in that it allows an unambiguous probability interpretation of an arbitrary state vector: the expansion coefficients of such vector in terms of the eigensystem are the probability amplitudes for finding the associated eigenvalues in a measurement.

Already in the early days of quantum mechanics the possible occurrence of non-Hermitian operators has been encountered. It was realised that an open system can be described by an effective non-Hermitian Hamiltonian where dissipation - complex eigenvalues with negative imaginary part - is brought about by a non-Hermitian term in the Hamiltonian. But even Hamiltonians that appear to be Hermitian naively can turn out to be non-Hermitian when boundary conditions are properly taken into account. Here we mention the Dirac Hamiltonian with the Coulomb potential  $-Z\alpha/r$  which fails to have a unique self-adjoint extension<sup>1</sup> if  $Z\alpha > 1$ , or the cranked anisotropic oscillator which has singularities associated with non-Hermitian properties, if the rotational frequency is equal to one of the oscillator frequencies<sup>2</sup>. In these and similar cases attempts have always been made to relate the onset of the change in mathematical structure with a physical effect: the “sparkling of the vacuum” in the case of the Dirac equation<sup>3</sup> for  $Z\alpha = 1$ , or the onset of an instability for the cranking model<sup>2</sup> if  $\Omega_{rot} = \omega_{ho}$ . As we see below, a new class of non-Hermitian Hamilto-

nians has given rise to different speculations, the critical review of which forms part of the present paper.

It has been established that Hamiltonians that are symmetric under  $\mathcal{PT}$  - the product of parity and time reversal<sup>4,5</sup> - can have a real spectrum<sup>6,7</sup> even though such operators need not be self-adjoint. In a host of papers devoted to the subject (see e.g.<sup>8</sup>, as well as this present Special Issue, for recent developments) the term *pseudo-Hermitian* operator was coined<sup>9</sup>, particularly related to issues concerning the reality of spectra. A property denoted as *quasi-Hermitian* was investigated in earlier work<sup>10</sup> where a complete and fully consistent quantum mechanical framework, based on non-Hermitian Hamiltonians treated in conjunction with other observables, had been established. (In essence this is pseudo-Hermiticity restricted to positive definite norms of states, as required by the probability interpretation which is central to quantum mechanics.)

The present paper revisits the relevant mathematical properties of quasi-Hermitian operators and critically discusses their possible physical implications. Particular emphasis is placed upon the metric associated with non-Hermitian operators and the related characterisation of the Hilbert space. The metric is introduced in the following section, with an emphasis on the notion of physical observables and their consistent introduction into a quantum mechanical framework built on a non-Hermitian Hamiltonian. In Sect. III we emphasise that the probability interpretation of quantum mechanics breaks down if care is not exercised in identifying physical observables within the quasi-Hermitian context. We also use the proper prescription for calculating transition probabilities with quasi-Hermitian observables to analyse when and why certain transition probabilities will not require a unique construction of the metric, while others do. In Sect. IV we illustrate these points by way of a few simple examples. This includes physical implications relating to the role of observables and the speculation about

the violation of the lower limit for transition times between orthogonal states of (Hermitian) observables (the “non-Hermitian brachistochrone problem”). A summary concludes the paper.

## II. THE METRIC AND OBSERVABLES

Even though the properties listed below have been stated and analysed in the literature<sup>9,10</sup> we here give a short recapitulation, with somewhat different emphasis, to make the paper self-contained.

While unbounded non-Hermitian operators constitute a difficult mathematical problem in general, there is the much simpler class that is well understood: the *quasi-Hermitian* operators. A non-Hermitian operator  $H \neq H^\dagger$  is called quasi-Hermitian if there exists a bounded Hermitian positive-definite operator  $\Theta$  that ensures the relation

$$\Theta H = H^\dagger \Theta. \quad (1)$$

The relation implies that  $H$  is similarly equivalent to a Hermitian operator, in fact the operator

$$h_S = S H S^{-1} \quad (2)$$

is Hermitian when  $S$  is the positive root of  $\Theta$ . The operator  $\Theta$  may be viewed as a metric characterising a different Hilbert space by defining the scalar product

$$\langle \cdot | \cdot \rangle_\Theta := \langle \cdot | \Theta \cdot \rangle \quad (3)$$

where  $\langle \cdot | \cdot \rangle$  is the usual scalar product, employing the  $L^2$ -metric being the identity. It is easily verified that (1) guarantees that the non-Hermitian  $H$  (with respect to the inner product  $\langle \cdot | \cdot \rangle$ ) is Hermitian with respect to  $\langle \cdot | \cdot \rangle_\Theta$ . Moreover, in view of (2) the spectrum of  $H$  is real. Note, however, that the eigenvectors  $|n\rangle$  obeying  $H|n\rangle = E_n|n\rangle$  are generally not orthogonal with respect to  $\langle \cdot | \cdot \rangle$ . There is, however, the bi-orthogonal system using the left hand eigenvectors  $\langle \tilde{n}|H = \langle \tilde{n}|E_n$  with  $\langle \tilde{n}|m\rangle = N_n \delta_{nm}$  which can be written as  $\langle n|\Theta m\rangle = N_n \delta_{nm}$ . In view of the discussion below we stress here the obvious: vectors being orthogonal with respect to a  $L^2$ -metric are not orthogonal when using the  $\Theta$ -metric and *vice versa*; the structure of a Hilbert space, that is the norm and orthogonality of its elements as well as the concept of Hermiticity is given by the definition of a scalar product.

The analysis of a quantum system described by a non-Hermitian Hamiltonian  $H$  usually confronts the construction and role of the metric  $\Theta$  by first focussing on the condition (1) for  $H$ . However, it should be emphasised that (1) does not uniquely determine  $\Theta$ . It is simple to see<sup>10</sup> that if  $\Theta$  is an acceptable metric determined by condition (1), so is  $\tilde{\Theta} = V\Theta$  with  $V$  any operator that commutes with  $H$ .  $\Theta$  is only uniquely determined when condition (1) holds for an *irreducible set* of operators  $A_i$ , all of which satisfy  $\Theta A_i = A_i^\dagger \Theta$  for the *same*  $\Theta$ . This also

determines those operators which may serve as physical observables (see<sup>10</sup>).

This observation is not only important to identify observables, but by implication also for the characterisation or labelling of states in terms of quantum numbers associated with observables, as well as for the proper calculation of transition matrix elements, as we proceed to illustrate in the following two sections.

To conclude this section we point out that the non-uniqueness of the metric as determined by a non-Hermitian (quasi-Hermitian) Hamiltonian *only*, leaves open the question of the definition (or construction) of other observables which may act consistently with it. Naturally, once a particular metric  $\Theta$  conforming to (1) has been chosen (rather than being *dictated* by an *a priori* consistent choice of a set of observables), then the observables can be obtained by *inverse* similarity transformation from standard observables, say  $a_i$  (such as  $x$  and  $p$ ). The operators so obtained,

$$A_i = S^{-1} a_i S \quad (4)$$

are then by construction quasi-Hermitian w.r.t. the metric  $\Theta$  which defines  $S$ , and accordingly qualify as observables.

## III. PROBABILITY INTERPRETATION AND MATRIX ELEMENTS

As indicated in the previous section, orthogonality of the eigenstates of a quasi-Hermitian operator is defined (and guaranteed) with respect to the inner product  $\langle \cdot | \cdot \rangle_\Theta := \langle \cdot | \Theta \cdot \rangle$ . Moreover, a given or chosen  $\Theta$ , compatible with (1), determines an irreducible set of observables  $A_i$ , and *vice versa*<sup>10</sup>.

It is almost pedantic, but nevertheless important in view of some recent discussions in the literature<sup>11,12,13</sup>, to emphasise the following. A cornerstone of quantum mechanics, the probability interpretation for measurement results of a given observable, rests on the orthogonality of its eigenstates. It is important to realise, therefore, that if an operator, typically an observable (say  $B$ ) Hermitian with respect to the standard inner product  $\langle \cdot | \cdot \rangle$ , is *not* from the irreducible set  $A_i$  determined by  $\Theta$ , then any standard calculation and interpretation of matrix elements involving eigenstates of  $B$ , would be meaningless within the context of the quantum mechanical system described by the non-Hermitian Hamiltonian  $H$  and observables  $A_i$ . This remains so even when  $B$  has a real spectrum (which of course does not depend on the Hilbert space inner product) and eigenstates which are orthogonal with respect to  $\langle \cdot | \cdot \rangle$ . The reason is simply that a consistent calculation of matrix elements (or probabilities) within the  $\Theta$  context requires the use of the inner product  $\langle \cdot | \cdot \rangle_\Theta := \langle \cdot | \Theta \cdot \rangle$ . Hence, absurd conclusions result upon using  $B$  as though it were a proper observable; e.g. denoting the eigenvalue problem for  $B$  as  $B|\beta_m\rangle = b_m|\beta_m\rangle$ , the probability of finding an eigenvalue

$b_m$  upon measurement of  $B$  in eigenstate  $|\beta_n\rangle$  ( $m \neq n$ ) is  $\langle\beta_m|\Theta|\beta_n\rangle$  which generally  $\neq 0$ . For a recent critical analysis of this point see<sup>14</sup>. (Similar arguments have recently also been put forward by Mostafazadeh<sup>15</sup>.)

Even when calculations are consistently performed, i.e. with due recognition of the metric operative within a given context, one may investigate the (in-)dependence of physical results on the choice of a metric determined by a non-Hermitian Hamiltonian as in (1), in particular from the point of view that  $\Theta$  is not uniquely determined by (1).

Let us accordingly consider an arbitrary member  $A$  from the set of observables which has determined  $\Theta$  uniquely. (It is worthwhile to stress that, at least in principle, either a given  $\Theta$  is chosen from among those that satisfy condition (1), which in turn uniquely determines which operators qualify as observables, or alternatively, the (non-Hermitian) Hamiltonian is supplemented by operators pre-chosen to be observables (and which form an irreducible set), which in turn pins down  $\Theta$  – see<sup>10</sup> for a full discussion). Here we simply assume that  $\Theta$  has been fixed and that  $A$  is an admissible observable. The prescription for calculating the transition probability  $P_{nm}(A)$  for the operator  $A$  between eigenstates  $|m\rangle$  and  $|n\rangle$  of the Hamiltonian  $H$  is unambiguous and yields the following:

$$\begin{aligned} P_{nm}(A) &= \frac{|\langle n|\Theta A|m\rangle|^2}{\langle n|\Theta|n\rangle\langle m|\Theta|m\rangle} \\ &= \frac{\langle n|\Theta A|m\rangle^* \langle n|\Theta A|m\rangle}{\langle n|\Theta|n\rangle\langle m|\Theta|m\rangle} \\ &= \frac{\langle m|\Theta A|n\rangle\langle n|\Theta A|m\rangle}{\langle n|\Theta|n\rangle\langle m|\Theta|m\rangle}. \end{aligned} \quad (5)$$

Here  $\langle n|$  is the bra or functional associated with  $|n\rangle$  through the original  $L^2$  inner product. In the second line we have used the fact that  $\Theta$  is Hermitian (in the original sense) and that  $A$  satisfies the quasi-Hermiticity relation  $\Theta A = A^\dagger \Theta$ .

Let us assume for the moment that the metric had not yet been uniquely fixed, e.g. when a full set of irreducible observables has not yet been specified, but with both  $H$  and  $A$  already included. In this case the calculation above may be repeated for another admissible metric  $\tilde{\Theta}$ , to give

$$\begin{aligned} P_{nm}(A) &= \frac{\langle m|\tilde{\Theta} A|n\rangle\langle n|\tilde{\Theta} A|m\rangle}{\langle n|\tilde{\Theta}|n\rangle\langle m|\tilde{\Theta}|m\rangle} \\ &= \frac{\langle m|V\Theta A|n\rangle\langle n|V\Theta A|m\rangle}{\langle n|V\Theta|n\rangle\langle m|V\Theta|m\rangle} \\ &= \frac{\langle m|\Theta A|n\rangle\langle n|\Theta A|m\rangle}{\langle n|\Theta|n\rangle\langle m|\Theta|m\rangle}, \end{aligned} \quad (6)$$

the same result as before! Here we have used the fact that  $V = \tilde{\Theta}\Theta^{-1}$  commutes with  $H$ , whence the states  $|n\rangle$  are simultaneous eigenstates of  $H$  and  $V$  (if there

are no degeneracies in the spectrum), yielding a cancellation of eigenvalues above and resulting in a transition probability which is *independent* of the metric!

However, it should immediately be cautioned that this is not a general result (see also<sup>10</sup>). It depends on (a) the absence of degeneracies in the spectrum, and more importantly (b) on the fact used above that the transition probability has been calculated with respect to eigenstates of  $H$  for an operator  $A$  that shares the property of quasi-Hermiticity with respect to a common metric (albeit not a unique one). Furthermore, it is clear that for general states (not eigenstates of  $H$  or another operator which shares in the property of quasi-Hermiticity) interference terms will appear which explicitly depend on the metric. If the metric had been chosen with respect to the Hamiltonian only, physical results will in general depend on the particular choice.

Writing the results (4) and (5) in the form

$$\begin{aligned} P_{nm}(A) &= \frac{\langle m|\Theta A|n\rangle\langle n|\Theta A|m\rangle}{\langle n|\Theta|n\rangle\langle m|\Theta|m\rangle} \\ &= \frac{\langle \tilde{m}|A|n\rangle\langle \tilde{n}|A|m\rangle}{\langle \tilde{n}|\tilde{n}\rangle\langle \tilde{m}|\tilde{m}\rangle} \end{aligned} \quad (7)$$

shows that a transition probability between eigenstates of  $H$  (or of any one of the observables) may be obtained by explicitly introducing both right and left eigenstates; choosing a particular bi-orthonormal normalisation  $\langle \tilde{n}|m\rangle = \langle n|\Theta m\rangle = \langle n|\Theta|m\rangle = N_n\delta_{nm}$  is equivalent to introducing a particular (and corresponding) metric or inner product.

The above point seems to have been overlooked from time to time in the literature, when the impression is given that the metric simply dictates a simultaneous transformation of operators and states, with no physical implications. It is also closely related to another simple, but important observation: when matrix elements or transition probabilities are being discussed or explicitly calculated within a quasi-Hermitian framework, the characterisation (or labelling) of such states can only be meaningfully carried out with reference to a set of operators (which should provide relevant quantum numbers) which are all observables and hence quasi-Hermitian with respect to the same metric. We again illustrate this point in section 5.

## IV. ILLUSTRATIVE EXAMPLES

### A. Non-uniqueness of the metric

The existence of a metric for a given non-Hermitian yet quasi-Hermitian Hamiltonian has been demonstrated in numerous examples<sup>10,16,17,18,19,20,21</sup>, and ways of constructing it have been given<sup>17,18,19,20,21,22,23</sup>. An important aspect that has already been emphasised in<sup>10</sup> and in the two previous sections seems to have been of lesser concern for some of the authors quoted. It is the fact

that there are many possible metric operators that ensure (1), usually a whole continuum. In other words, there are many ways of finding a Hermitian Hamiltonian  $h_S$ , each associated with a different metric, i.e. each invoking a different Hilbert space. The physical implications are discussed in the following section. Here we focus upon some formal issues.

A simple example<sup>21</sup> may demonstrate the essential points. Consider the toy Hamiltonian

$$H = \omega(a^\dagger a + \frac{1}{2}) + \alpha a^2 + \beta a^{\dagger 2} \quad (8)$$

with  $a$  the usual boson operators. For  $\alpha \neq \beta$  the Hamiltonian is manifestly non-Hermitian. The spectrum is given by  $E_n = (n + 1/2)\Omega$  with  $\Omega = \sqrt{\omega^2 - 4\alpha\beta}$  which is real for  $\omega^2 > 4\alpha\beta$ . For real  $\Omega$  a continuum of choices can be found for the metric and can be parametrised by the real parameter  $z \in [-1, 1]$  yielding

$$h_{S(z)} = \Omega(b_z^\dagger b_z + \frac{1}{2}) \equiv \frac{1}{2}(\mu(z)p^2 + \nu(z)x^2). \quad (9)$$

with  $\mu(z)\nu(z) = \Omega^2$  identically in  $z$ . The metric by which this is achieved is given by<sup>21</sup>

$$\Theta(z) = \left( \frac{\alpha + \beta - \omega z + (\alpha - \beta)\sqrt{1 - z^2}}{\alpha + \beta - \omega z - (\alpha - \beta)\sqrt{1 - z^2}} \right)^{\frac{p^2(1-z) + \omega^2 x^2(1+z)}{4\omega\sqrt{1-z^2}}}. \quad (10)$$

up to a constant. Being faced with a continuous variety of Hilbert spaces  $\mathcal{H}_z$  the obvious question is now for Hermitian operators other than  $H$  (recall that  $H$  is Hermitian in  $\mathcal{H}_z$  for any  $z$ ). The answer is readily given by (10) and will, of course, depend on  $z$ . In fact, seeking the operator  $O$  such that

$$\Theta(z)O = O^\dagger\Theta(z)$$

there is only the combination  $O(z) = p^2(1-z) + \omega^2 x^2(1+z)$  fulfilling this requirement. Note that neither the momentum nor the position operator remains Hermitian except if  $z = -1$  or  $z = 1$ , respectively; for  $z = 0$  we identify the number operator  $a^\dagger a \sim p^2 + \omega^2 x^2$  as being Hermitian.

This example nicely demonstrates the point made in<sup>10</sup>: the metric can be defined uniquely if operators in addition to  $H$  are required to be quasi-Hermitian. In general the additional operators have to form an irreducible set together with  $H$ , in the example above there is just one more, namely  $O(z)$ .

While the expressions (9) and (10) are valid only if  $\Omega$  is real, there are further restrictions from the requirement that  $\Theta$  be bounded and strictly positive. Yet the numerator or denominator of (10) vanishes for

$$z_{\pm} = \frac{(\alpha + \beta)\omega \pm (\alpha - \beta)\Omega}{\omega^2 + (\alpha - \beta)^2}, \quad (11)$$

respectively. For  $z$  between  $z_-$  and  $z_+$  the metric is ill defined and  $h_S$  is not the Hermitian equivalent of  $H$ . These singularities are spurious, i.e. they are not intrinsic

to the problem and can be removed<sup>19</sup>. In the example given the substitution of  $z$  by  $-z$  achieves this goal but at the expense of trading in spurious singularities elsewhere. The conclusion is that a metric that is globally free of singularities cannot be found<sup>19</sup>.

There are other more serious types of singularities as they are intrinsic to the problem and cannot be removed. They always render the metric undefined. These are the exceptional points (EP)<sup>24,25,26</sup> occurring - in the example - for  $\Omega = 0$ , the point where levels coalesce and the spectrum becomes non-real. We return to these singularities in the following section; they are claimed to have physical consequences in the context of  $\mathcal{PT}$ -symmetric Hamiltonians.

## B. Brachistochronous behaviour

The study of quasi-Hermitian operators received a strong boost when it was realised that Hamiltonians that are symmetric under  $\mathcal{PT}$  can have a real spectrum, while not being necessarily Hermitian<sup>4,5</sup>. The question as to physical implications of this more general viewpoint of a formulation of quantum mechanics, however, remains open.

In<sup>11,27,28</sup>  $2 \times 2$  quasi-Hermitian matrix Hamiltonians are considered, in particular the  $\mathcal{PT}$ -symmetric Hamiltonian<sup>11</sup>

$$H = \begin{pmatrix} re^{i\theta} & s \\ s & re^{-i\theta} \end{pmatrix}, \quad (12)$$

with  $r, s, \theta$  real. It has the eigenvalues  $E_{\pm} = r \cos \theta \pm \sqrt{s^2 - r^2 \sin^2 \theta}$  and the unnormalised eigenvectors

$$|E_{-}\rangle = \begin{pmatrix} -e^{-i\alpha} \\ 1 \end{pmatrix} \quad |E_{+}\rangle = \begin{pmatrix} e^{i\alpha} \\ 1 \end{pmatrix} \quad (13)$$

where  $\alpha$  is defined by  $\sin \alpha = r/s \times \sin \theta$ .

This example nicely demonstrates

- (a) some uniform features of a  $\mathcal{PT}$ -symmetric Hamiltonian;
- (b) spontaneous symmetry breaking at an EP, including all properties inherent to an EP.

(a) The spectrum is real when  $|s| > |r \sin \theta|$ , for this parameter range the auxiliary parameter  $\alpha$  is real,  $\alpha \in (-\pi/2, \pi/2)$ , and the two eigenfunctions are themselves eigenfunctions of the  $\mathcal{PT}$  operator. The metric can be chosen as

$$\Theta = \begin{pmatrix} 1 & -i \sin \alpha \\ i \sin \alpha & 1 \end{pmatrix} \quad (14)$$

being Hermitian and positive in the range  $\alpha \in (-\pi/2, \pi/2)$ . (The general form for  $\Theta$  is introduced below, but this choice already enables us to make some salient points.) We mention that the Hamiltonian (12)

when transformed by the similarity transformation  $S = \Theta^{1/2}$  assumes the form

$$h = SHS^{-1} = \begin{pmatrix} r \cos \theta & \sqrt{s^2 - r^2 \sin^2 \theta} \\ \sqrt{s^2 - r^2 \sin^2 \theta} & r \cos \theta \end{pmatrix}$$

which is manifestly Hermitian. Note that this choice of the metric implies that  $\sigma_y$  is quasi-Hermitian, i.e. an observable, but not the  $\sigma_z$ , as is implied in<sup>11</sup>.

(b) When  $s = \pm r \sin \theta$ , that is when  $\alpha = \pm \pi/2$ , the eigenvalues coalesce and we encounter all the properties of an EP. That is

(i)  $H$  cannot be diagonalised, its Jordan form is

$$H = \begin{pmatrix} r \cos \theta & 1 \\ 0 & r \cos \theta \end{pmatrix},$$

(ii) the eigenvalues are connected by a square root branch point,

(iii) the eigenvectors become aligned and assume both the form

$$\begin{pmatrix} i \\ 1 \end{pmatrix}$$

and they cannot be normalised as their norm vanishes, and

(iv) the metric is no longer positive-definite.

Beyond that point, when  $|s| < |r \sin \theta|$ , the eigenvalues are complex, the eigenvectors are no longer eigenstates of the  $\mathcal{PT}$  operator as  $\alpha$  is complex.

In particular in view of the alignment of the eigenvectors, meaning physically that there is - at the singularity - just one state, one cannot speak of a transition. In other words, the concept of a “transition time” becomes meaningless.

### C. A generalisation

For the sake of completeness we give here the general form of the metric obeying (1) for the Hamiltonian (12). If  $\sin \alpha < 1$  we may choose

$$\Theta = \begin{pmatrix} 1 & \sin \gamma - i \sin \alpha \\ \sin \gamma + i \sin \alpha & 1 \end{pmatrix} \quad (15)$$

using the additional free parameter  $\gamma$  which must obey the constraint

$$\sin^2 \gamma + \sin^2 \alpha < 1 \quad (16)$$

to ensure that  $\Theta$  is positive-definite. The Hermitian Hamiltonian generated by  $S = \Theta^{1/2}$  reads now

$$h = SHS^{-1} = \begin{pmatrix} r \cos \theta & f(r, s, \theta, \gamma) \\ \bar{f}(r, s, \theta, \gamma) & r \cos \theta \end{pmatrix} \quad (17)$$

where

$$f(r, s, \theta, \gamma) = \frac{s \sin \gamma + ir/s \sin \theta \sqrt{s^2 \cos^2 \gamma - r^2 \sin^2 \theta}}{\sin \gamma + ir/s \sin \theta}$$

and  $\bar{f}$  denotes the complex conjugate. Of course, it is  $f(r, s, \theta, 0) = \sqrt{s^2 - r^2 \sin^2 \theta}$  and the eigenvalues of (17) are still given by those of (12). This generalisation simply confirms that there is (i) a continuum of choices for a metric, and (ii) spurious singularities can occur depending on the choice of the metric. In fact, when  $\sin \gamma = \pm \sqrt{1 - \sin^2 \alpha}$  the metric ceases to be positive-definite. When (16) is invalidated,  $S = \Theta^{1/2}$  can no longer be Hermitian, as a consequence (17) is not Hermitian either. Yet a different choice for  $\gamma$  can remove that deficiency. Note, however, even when  $\gamma$  is chosen to be zero, the EP ( $\sin \alpha = \pm 1$ ), where the levels *and* the eigenfunctions coalesce, is intrinsic to the problem: this singularity persists.

Here we mention that, while for  $\sin \alpha = 1$  the Hamiltonian (12) cannot be diagonalised, its hermitised “counterpart” is diagonal and has a genuine degeneracy. However, the two operators are no longer similarly equivalent since  $S^{-1} = \Theta^{-1/2}$  does not even exist.

Concerning the question of observables, the general form for the metric clearly shows that  $\sigma_z$  can never be an observable for (12). In fact, for this to hold, the condition  $\Theta \sigma_z = \sigma_z \Theta$  had to be obeyed. As  $\Theta$  has the general form  $\Theta = 1 + \sin \gamma \sigma_x + \sin \alpha \sigma_y$  this can only be for  $\alpha = \gamma = 0$  reducing the problem trivially to (12) being Hermitian. By the same reasoning, in general, only the combination  $\sin \gamma \sigma_x + \sin \alpha \sigma_y$  is an observable within the allowed range of the parameters. Using the appropriate metric  $\Theta$ , not only are the expectation values of  $\sigma_z$  complex in general but the probability interpretation becomes inconsistent. In short, under the regime of (12) (with  $\alpha \neq 0$ )  $\sigma_z$  is not an observable. Rather, the  $z$ -component of spin must be described by  $\Sigma_z = S^{-1} \sigma_z S$ .

### D. Classical limit

We stress that even the classical limit of a non-Hermitian  $\mathcal{PT}$ -symmetric Hamiltonian can depend on the metric chosen<sup>21</sup>. In fact, the classical limit of (9) is obvious and so is the classical expression for the energy. The  $z$ -dependence of the mass term persists and we obtain  $E_{\text{class}} = A^2 \Omega^2 / (2\mu(z))$  with  $A$  being the amplitude of the classical oscillation.

## V. SUMMARY

Virtually all problems and questions raised in the present paper become self-evident or obsolete if traditional quantum mechanics is being adhered to. Yet, recent developments considering quasi-Hermitian Hamiltonians, in particular in the context of  $\mathcal{PT}$ -symmetry, jus-

tify in principle a possible formal extension of the theoretical framework. However, the consequences (and possible pitfalls) need to be scrutinised afresh. This is the subject of the present paper.

While there seems to be agreement in the literature that consideration of quasi-Hermitian Hamiltonians cannot *a priori* be excluded on logical or physical grounds, the non-trivial (non-unity) metric that comes with it to guarantee a consistent framework is not unique. To be precise, only when the choice is made of an irreducible set of operators  $A_i$  satisfying  $\Theta A_i = A_i^\dagger \Theta$  is the metric  $\Theta$  fixed.

The examples discussed above illustrate the general points already made in Sects. II and III: (i) once a quasi-Hermitian Hamiltonian is given, there is some restriction from the start about which traditional observable can (or should) be chosen to remain invariant under (4), and (ii) the set  $A_i$  can be a combination of traditional observables implying one or more continuous parameters. In fact,  $\sigma_z$  cannot be chosen for the Hamiltonian (12), and only  $(1-z)p^2 + (1+z)x^2$  is a possible choice for (8). These results have rather stringent consequences. Assuming a physical setting can be modelled by (12), the  $z$ -component of the spin cannot be described  $\sigma_z$ ; it must in fact be described by  $\Sigma_z = S^{-1}\sigma_z S$ . Similarly, the associated orthogonal states describing “spin up” and “spin down”, must be the eigenstates of  $\Sigma_z$ . Furthermore, certain quantities of physical interest, such as probabilities and transition amplitudes, will in general depend on the continuous parameter, that is on  $\gamma$  for (12) and on  $z$  for (8). Once the choice (or construction) of an irreducible set of observables has been completed, physical quantities will be fixed, but, as discussed in Sect. III some of them will depend on the metric implied by that choice (or construction).

In addition, in contrast to traditionally Hermitian Hamiltonians, singularities can and generically will occur as part of the real spectrum. The EPs signal usually the points in parameter space where (i) the metric be-

comes singular, and where (ii) the spectrum ceases to be real. These points of coalescence of spectrum and eigenfunctions can, because of their specific singular nature, lead to misinterpretations. The conclusions drawn in the literature about the Hamiltonian (12) are doubtful for two reasons. Firstly, the approach of the EP, where the eigenspace of (12) is no longer two-dimensional, requires particularly cautious analysis. In fact, while it is true that at a distance from the EP, there is a two-dimensional bi-orthogonal eigensystem, the normalised vectors tend to infinity and become aligned when the limit is attained. To translate this into “transition time going toward zero” means deviating from quantum mechanical interpretation where only transitions between strictly orthogonal and normalisable states can be considered unambiguously<sup>14</sup>. Moreover, since  $\sigma_z$  is no valid observable, the spin flip claimed to be the indicator of a “brachistochronous” transition cannot be observed. This apparently counter-intuitive statement - after all, can’t we always measure a spin projection? - needs explanation: yes, we can, but *not* in terms of  $\sigma_z$  when a system should evolve under the regime of a Hamiltonian as given by (12). An analysis concerning the  $z$ -component of spin should be carried out in terms of  $\Sigma_z = S^{-1}\sigma_z S$  and its eigenstates, in which case the known Hermitian brachistochrone result is again obtained<sup>15</sup>.

We feel that the efforts to go beyond the framework of traditional quantum mechanics has certainly further enhanced our understanding of it. However, as long as no guidance from some experiments is at hand, the ambiguities presented here cannot be removed. The non-uniqueness of the metric and the physical significance of its singularities require guidance by an actual physical situation. We only mention that inconsistencies persist when attempts are made to consider switching from one metric to another, such as by a time-dependent metric<sup>29</sup>. Such attempts imply changing the underlying Hilbert spaces, hence any result can be construed.

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- <sup>1</sup> Rafelski J, Fulcher L P and Klein A 1978, Phys. Rep. **38** 227
  - <sup>2</sup> Heiss W D and Nazmitdinov R G 2007, J. Phys. A: Math. Theor. **40** 9475
  - <sup>3</sup> Greiner W 1985, in Lecture Notes in Physics **231**, W D Heiss (Ed.) (Heidelberg: Springer)
  - <sup>4</sup> Bender C M and Boettcher S 1998, Phys. Rev. Lett. **80** 4243
  - <sup>5</sup> Bender C M 2007, Rep. Prog. Phys. **70** 947
  - <sup>6</sup> Dorey P, Dunning C and Tateo R 2001, J. Phys. A: Math. Gen. **34** 5679
  - <sup>7</sup> Shin K C 2002, Commun. Math. Phys. **229** 543
  - <sup>8</sup> Geyer H B, Heiss W D and Znojil M (Eds.) 2006, J. Phys. A: Math. Gen **39**, No. 32 (Special issue on *The Physics of Non-Hermitian Operators*)
  - <sup>9</sup> Mostafazadeh A 2002, J. Math. Phys. **43** 205; *ibid* **43** 2814; *ibid* **43** 3944
  - <sup>10</sup> Scholtz F G, Geyer H B and Hahne F J W 1992, Ann. Phys. (N.Y.) **213** 74
  - <sup>11</sup> Bender C M, Brody D C, Jones, H F and Meister B K 2007, Phys. Rev. Lett. **98** 040403
  - <sup>12</sup> Assis P E G and Fring A 2007, e-print [arXiv:0703254 \[quant-ph\]](#)
  - <sup>13</sup> Günther U and Samsonov B F 2007, e-print [arXiv:0709.0483 \[quant-ph\]](#)
  - <sup>14</sup> W H Zurek, e-print [arXiv:0703160 \[quant-ph\]](#)
  - <sup>15</sup> Mostafazadeh A 2007, Phys. Rev. Lett. **99** 130502
  - <sup>16</sup> Geyer H B, Snyman I and Scholtz F G 2004, Czech. J. Phys. **54** 1069
  - <sup>17</sup> Jones H F 2005, J. Phys. A: Math. Gen. **38** 1741
  - <sup>18</sup> Scholtz F G, Geyer H B 2006, Phys. Lett. B **634** 84
  - <sup>19</sup> Scholtz F G, Geyer H B 2006, J. Phys. A: Math. Gen. **39** 10189
  - <sup>20</sup> Mostafazadeh A 2006, J. Phys. A: Math. Gen. **39** 10171

- <sup>21</sup> Musumbu D P, Geyer H B and Heiss W D 2007, J. Phys. A: Math. Theor. **40**, F75
- <sup>22</sup> Fring A and Figueira de Morisson Faria C 2006, Czech. J. Phys. **56**, 899
- <sup>23</sup> Mostafazadeh A 2006, J. Math. Phys. **47**, 072103
- <sup>24</sup> Kato T 1976, *Perturbation Theory for Linear Operators* 2nd edn (Heidelberg: Springer)
- <sup>25</sup> Heiss W D 2004, Czech. J. Phys. **54** 1091
- <sup>26</sup> Heiss W D 2006, J. Phys. A: Math. Gen. **39** 10081
- <sup>27</sup> Znojil M, Geyer H B 2006, Phys. Lett. B **640** 52; *ibid* **649** 494
- <sup>28</sup> Mostafazadeh A and Ozcelik S 2006, Turk J. Phys. **30**, 437
- <sup>29</sup> Mostafazadeh A 2007, Phys. Lett. B **650** 208
- <sup>30</sup> Strictly speaking they should be self-adjoint operators. Hermiticity only requires  $(\phi, A\psi) = (A\phi, \psi)$ , while self-adjointness requires that the domains of  $A$  and  $A^\dagger$  also coincide, i.e., self-adjointness is a strict operator equality  $A = A^\dagger$